Evanescent coupling in a waveguide fluoroimmunosensor

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ABSTRACT

A key factor in the analysis of evanescently-coupled optical sensors, such as the planar waveguide immunosensor analyzed here, is the efficiency of coupling between the optical waveguide modes and the fluorescent sources located on the surface of the waveguide. This is an important parameter in determining the sensor's sensitivity to the analyte. We calculate this efficiency for several different sensor configurations using the finite-difference time-domain (FDTD) numerical technique, and find that the efficiency of one-way coupling can vary widely depending upon the fluorescent source polarization, phase, and distance from the surface, as well as the waveguide mode number and thickness. In particular, we find that when the layer containing the fluorescent molecules is uniform in refractive index, the coupling efficiency is larger than when the local environment possesses an irregular index.

1. INTRODUCTION

Fluoroimmunosensors detect the amount of antigen in a fluid sample by exciting and detecting fluorescence in a fluorophore/label attached to either the antibody or a duplicate antigen.[1] In waveguide immunosensors, the excitation and often collection of the fluorescence is via the evanescent tails of the waveguide modes that stretch into the fluid region containing the antibodies and bound antigens on the surface of the guide. The percentage of overlap between the electric field in the evanescent tail and the fluorescent molecule determines how much coupling occurs between the molecules and the optical waveguide modes, but this is often difficult to calculate theoretically because of variations in the evanescent penetration depth due to the particular mode structure of the guide and because of different arrangements of the molecules on the surface, such as their orientation and the nature of the surrounding media.

We use a relatively new numerical analysis technique called finite-difference time-domain[2] (FDTD) to calculate the coupling between the fluorescent molecules and the waveguide modes. In our model, the fluorophores are represented by electric dipoles near the surface of the waveguide, and the percentage of total fluorescent power radiated by these sources that is trapped inside the waveguide as guided modes gives a measure of the one-way coupling, or collection efficiency.[3] The reciprocal question of excitation efficiency, that is, the amount of laser power inside the guide which is useful in exciting the fluorophores, is expected to be of the same order of magnitude by the principle of reciprocity.

2. MODEL OF WAVEGUIDE AND SOURCES

The two-dimensional model for the theoretical analysis is shown in Fig. 1. The waveguide is modeled as a planar guide of thickness d with an index of refraction n; for the test cases reported in this paper, the index of the guide is taken to be similar to polystyrene (n=1.60) and the thickness is set to d=0.4 μm. The wavelength of the emission is 488 nm. This makes the normalized frequency parameter of the guide V=3.377, so the guide is single-mode and will support only the lowest order TM_0 mode.[4] The region above the guide is assumed to be water with an index n=1.33, and the substrate below the guide is assumed to be silica with an index of n=1.46. Both superstrate and substrate regions extend to infinity in the model, due to the radiating boundary conditions (absorbing boundary conditions) which are imposed around the entire outer boundary of the model.

The FDTD algorithm effectively solves Maxwell's equations in finite-difference form over a gridwork of small cells (Yee cells) which makes up the model space. In each cell, the electric field value and magnetic field value then yield the Poynting vector power density passing through that cell.

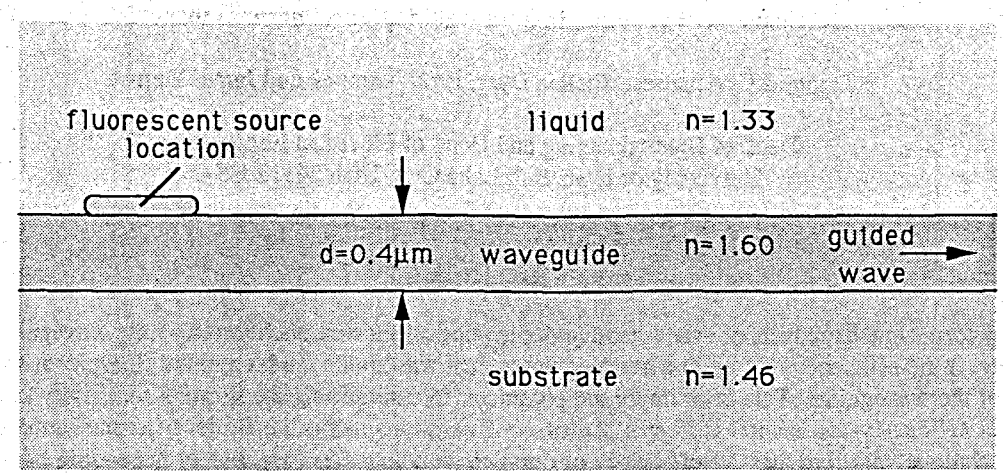

Fig. 1. Two-dimensional model of the waveguide sensor configuration analyzed, with the fluorescent sources located on the top surface of the guide.

The fluorescent molecules are modeled as electric dipole sources in various source cells located on top of the waveguide. The particular orientation (polarization) of the electric dipoles, as well as their relative phases, take on different values for the various cases analyzed in this study. In addition, the index of refraction of the local layer immediately surrounding the fluorescent sources is modeled as either irregular or as uniform, in order to determine the effect of the uniformity of this layer on the efficiency of coupling.

The coupling efficiency is then found in the following way: After the fields are found in each cell in the model grid by the FDTD method, the components of the Poynting vectors normal to the outside boundaries in all the cells around the periphery of the model are calculated. By adding these components from every cell around the entire periphery, a value for the total radiated power P_r from the sources is obtained. Then, the normal components of the Poynting vectors for just those cells located inside the two ends of the waveguide are added to give a measure of the power P_g trapped in the waveguide. The ratio

$$R = P_g / P_r$$

is an indication of the coupling efficiency between the radiating dipoles and the waveguide modes. Note that the guided power P_g (and the ratio R) includes the power travelling in both directions in the waveguide for this analysis.

3. RESULTS FOR DIFFERENT SOURCE CONFIGURATIONS

We have analyzed several different combinations of source polarizations, number of dipoles, relative phases, and waveguide characteristics. One simple configuration of a single fluorescent dipole is shown in Fig. 2. Here the dipole is polarized in a direction normal to the waveguide, which is the dominant field direction for the evanescent tail of the TM_0 mode. The FDTD calculations show that the coupling ratio is R=0.12, which means that 12% of the total radiated fluorescence is trapped in the guided modes.

A more interesting case is shown in the next two figures. Figure 3 shows a source configuration of several (ten) dipoles at random locations, i.e., with random spaces between the individual dipoles. The spaces between dipoles are assumed to contain the surrounding fluid (water) and therefore these cells have an index of n=1.33. On the other hand, those cells which contain a dipole source are given an index of n=1.5, simulating the index of the antibodies to which the fluorescent labels are attached. Therefore, this configuration models an irregular protein layer. The polarizations of the

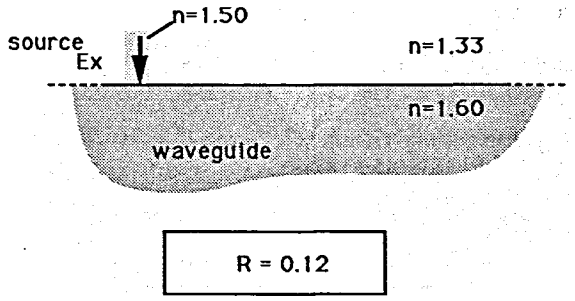

Fig. 2. Single dipole source polarized perpendicular to the waveguide surface. The coupling ratio is 0.12.

electric field dipoles are randomized between the two extremes of perpendicular and parallel orientations to simulate random molecule orientation. The relative phase distribution among the dipoles--a very important parameter which determines the amount of constructive or destructive interference which takes place between the individual contributions from the dipoles--has been given twelve different random profiles, and the mean of the coupling ratio is statistically determined for this ensemble of profiles. For the case of the irregular layer in Fig. 3, R=0.217.

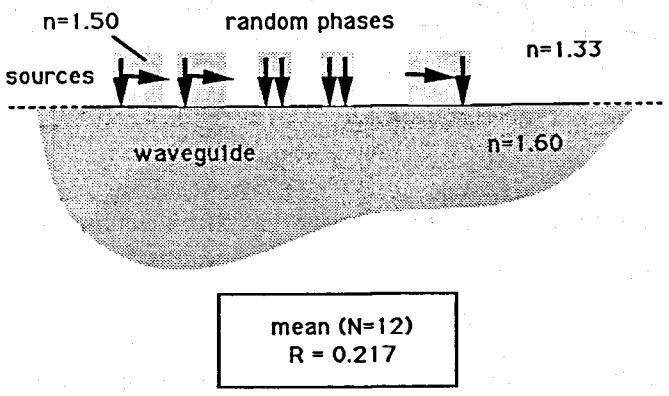

Fig. 3. Multiple dipole sources, with the spaces between dipoles filled with water (n=1.33), giving a layer with irregular refractive index. The mean coupling ratio, for twelve different phase distributions, is R=0.217.

Figure 4 shows the same multiple-source configuration as Fig. 3, except that the spaces between the dipoles are assumed to be filled with the same higher index material (proteins, or antigens /antibodies) as immediately surrounds the dipoles. Therefore this case models a homogeneous protein layer uniformly on top of the guide, as would happen if non-fluorescent proteins filled in the spaces between the fluorescent proteins. Again, an ensemble of twelve different phase distributions has been analyzed, with a mean coupling ratio of R=0.242.

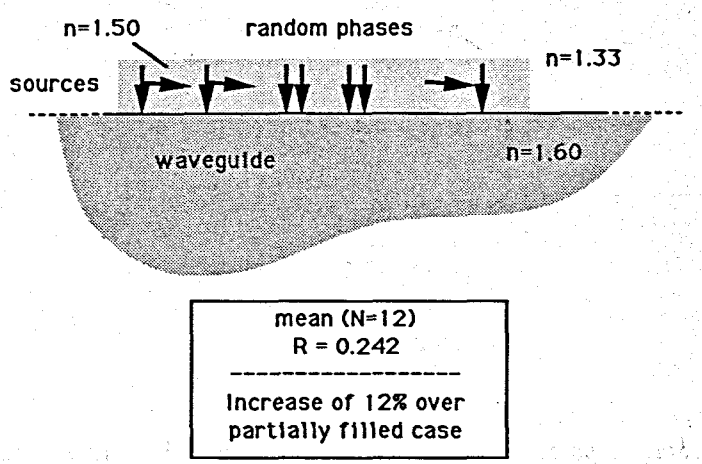

Fig. 4. The same multiple dipole sources as seen in Fig. 3, except the spaces between dipoles are filled with protein (n=1.50), providing a uniform layer. The mean coupling ratio, for twelve different phase distributions, is R=0.242.

4. DISCUSSION AND CONCLUSIONS

An appreciable amount of power radiated by fluorescent sources located on top of a waveguide may be coupled into the guided modes. The exact amount depends upon the polarization and number of the sources as well as the local environment surrounding the sources. The case analyzed in Figs. 3 and 4 applies to the situation where non-fluorescent proteins (such as antigens without fluorescent labels) may fill in the spaces between the fluorescent proteins, making the layer more uniform in refractive index. The FDTD analysis suggests that a greater coupling ratio (an increase of 12% in the models of Figs. 3 and 4) will result when the layer is uniform, compared to an inhomogeneous layer. This may be an explanation for the experimental observation of increased collected fluorescence intensity when non-labeled proteins are introduced onto the surface of a fiberoptic sensor for which the concentration of labeled proteins remains unchanged.[5]

From the above results it can be seen that the FDTD method provides an accurate technique for analyzing various optical sensor configurations, being especially sensitive to near-field effects and complex geometries.

5. ACKNOWLEDGMENTS

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6. REFERENCES

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